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# CHEMICAL TRANSPORT, HUMAN EXPOSURE, AND HEALTH RISK: A MULTIMEDIA APPROACH


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# CHEMICAL TRANSPORT, HUMAN EXPOSURE, AND HEALTH RISK: A MULTIMEDIA APPROACH

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ABSTRACT

Multimedia models simulate the transport and transformation of chemicals in multiple environmental media, such as air, water, soil, biota, and sediments. Such models are useful for developing a macroscopic view of environmental chemistry. In this paper we explore the use of multimedia models in risk assessment. We begin with a discussion of how multimedia models can be used to enhance the risk-assessment/management process. This is followed by a description of a multimedia model, called GEOTOX, that uses physicochemical and landscape properties to estimate the intermedia transport rates of a chemical. These rates are used to estimate chemical concentrations in the air, water, soil, and food of a representative or generic environment. We use these concentrations in exposure-pathway models to calculate quantities absorbed by humans; then, dose-response data are used to estimate health risks. We illustrate the use of these models in a risk-based screening procedure for hazardous chemicals. The paper concludes with a discussion of the limits and capabilities of this approach.

## INTRODUCTION

Cross-media or multimedia pollution has been attracting the interest of environmental scientists because of recent efforts to control groundwater contamination and acid rain. Both of these problems result from a pollutant that is generated in one medium and then contaminates another. Solvents buried in landfills, for example, move from soil to become potentially toxic pollutants in air or in ground and surface water. We have developed a multimedia compartment model, called GEOTOX, that simulates the transport and transformation of chemicals through multiple environmental media: air, water, biota, soils, sediments, and ground water.[1] Using this model with the appropriate landscape and chemical properties, we determine how a given chemical distributes itself among the different environmental media. The resulting environmental concentrations are combined with an exposure model and health effects data to estimate potential human health risks. We have used this model to screen out the important hazardous chemical residuals that result from the destruction of waste ordnance.[2] However, this approach can be used to evaluate the residuals from a number of industrial technologies.

There is nothing novel in the concept that the environment is a system composed of air, water, biota, and soil compartments through which elements and pollutants cycle. This approach is fundamental to the science of radioecology. Moreover, the U.S. Environmental Protection Agency (EPA) was created in 1970 in an attempt to match pollution-control efforts more closely with the growing perception of the environment as a single, interconnected system. But in order to reach cleanup goals rapidly, amendments to air and water laws reinforced a contrary focus on separate controls for air and water pollutants. Now, over a decade later, interest in a more unified approach to pollution control is emerging again.

Attempts to organize pollution-transport evaluations to take into account the interrelationship of air, water, and soil pollution have been labeled <u>integrated</u>, <u>intermedia</u>, <u>holistic</u>, <u>multimedia</u>, and <u>cross-media</u>.[3-10] Figure 1 illustrates such a view of the environment. These terms emphasize the importance of the transfer of pollutants among the media. In the sense of a "channel" or "vehicle," <u>medium</u> is a useful term to describe the function of air, water, and soil in relation to pollutants. We use the term <u>multimedia</u> to refer to an analysis that accounts for the overall behavior of a pollutant in air, water, and soil.

There are now some 66,000 chemicals in commercial use.[11] For many of these compounds, relatively little is known about how they behave in the environment or about their potential effects. However, it is known that some chemicals can have serious adverse effects on humans at very low levels of exposure. Thus, managing the potential health risks of industrial residuals requires analysis of the transport, transformation, and human uptake of an ever-increasing list of pollutants. The very magnitude of this list precludes a detailed assessment of all the potential impacts of every chemical in the marketplace. Nonetheless, it is possible to acquire sufficient data about most chemicals to perform preliminary screening studies that identify important compounds and set priorities for expanding the environmental data base. It is this situation that prompted the development of the GEOTOX model. This model was developed to provide a simple, yet comprehensive, picture of the dynamic behavior of chemicals in the environment.

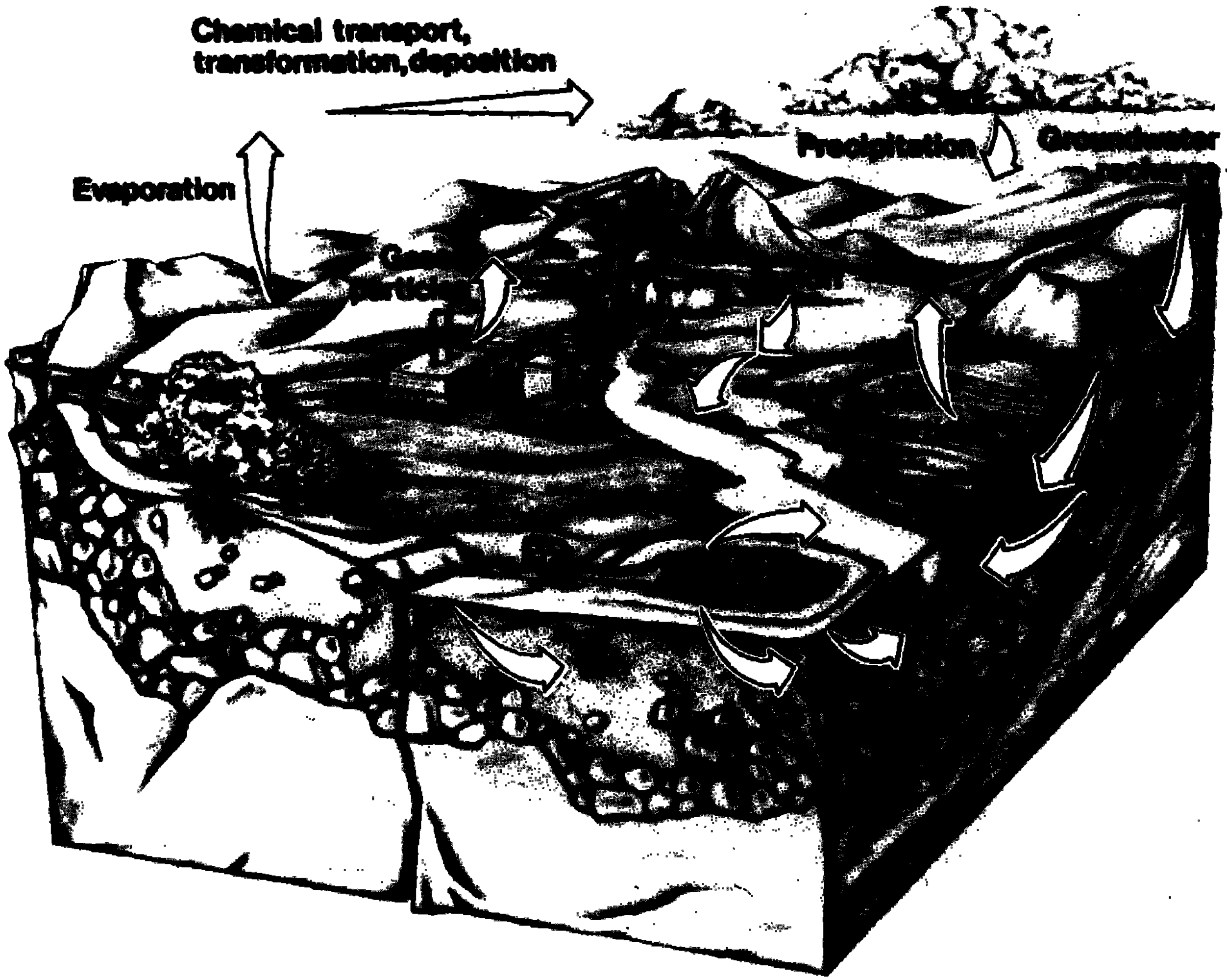




Figure 1. An illustration of the multimedia approach showing chemical transport and transformation.

This paper is divided into four sections. In the first section, we describe the GEOTOX model and how it is used to determine environmental concentrations and human exposure. In the next section, we discuss the use of multimedia transport models in risk assessment/management. In the third section, we provide an application of the GEOTOX model for ranking six chemicals. In the final section of the paper, conclusions are presented.

## GEOTOX: A MULTIMEDIA COMPARTMENT MODEL

Compartmental systems consist of a finite number of homogeneous, lumped subsystems, called compartments, that exchange physical quantities such as thermal energy, chemical contaminants, or nutrients with each other or with the external environment in such a way that the quantities or concentrations of material within the compartments may be described by a set of first-order, ordinary differential equations. A compartmental system may be used to model either the transport kinetics of one substance or of two or more substances (such as a radionuclide and its decay products).

GEOTOX is a computer program that organizes and solves the set of first-order differential equations that describe the transient mass balance of a chemical in a multicompartment environment. The program was developed originally at the University of California, Los Angeles, for ranking the potential health risks of toxic metals and radionuclides in the global landscape.[12] The current version was modified at Lawrence Livermore National Laboratory to also handle organic compounds. GEOTOX was originally coded to run on mainframe computers, but the current version was compiled in Microsoft® Fortran and runs on a personal computer.

A multimedia compartment model suitable for risk-assessment/management studies must meet several criteria. Among them we have identified the following:

(1) have the ability to handle organic chemicals, trace elements, and radionuclides;

(2) be simple enough to allow multiple runs for sensitivity studies;

(3) the ability to link environmental concentrations with exposure pathways to calculate human intake;

(4) be flexible enough to handle steady-state and dynamic situations; and

(5) can be altered easily to simulate different types of ecoregions.

There is currently no model that fully satisfies all of these criteria. However, in the process of modifying the GEOTOX model, we use these criteria as objectives to be met as the program evolves. The current version of GEOTOX performs two major tasks: (1) it projects the transport and transformation of chemicals within a multimedia environment and (2) estimates contaminant doses to humans. The chemical-transport model uses landscape data and physicochemical properties to determine the distribution and concentration of chemicals among compartments such as air, water, and soil. Environmental concentrations are linked to human exposures and health effects using an exposure model that accounts for intake through inhalation, consumption of food and water, and dermal absorption.

The choice of compartment structure requires a balance between two competing concepts, simplicity of the model and the value of the information provided. Because the model is required to provide a framework for assessing the environmental fate of chemical species, it should, even in its most simple form, include at least three compartments: air, water, and soil. However, because much of the exchange of chemicals occurs at interfaces such as soil/water, soil/atmosphere, and water/sediment and because of the role of the surface biota as a possible reservoir for chemicals, we choose to use a minimum of eight compartments. These are atmospheric gas, atmospheric particles, land biota, upper soil layer, lower soil layer, groundwater zone, surface water, and surface-water bottom sediments.

Each compartment is composed of from one to as many as three phases: solid, liquid, and/or gas. A compartment is described by its total mass, total volume, solid mass, liquid mass, and gas mass. Mass flows among the compartments consist of solid flows and liquid phase flows. Figure 2 illustrates the conceptual layout of the environment as it is viewed by the eight-compartment GEOTOX model. In the paragraphs that follow, we describe how the mass, volume, and liquid and solid exchanges among the compartments are quantified.

## Calculation of Transfer Rates and Decay Constants

Chemical exchange among compartments occurs by advection in the solid phase, advection in the liquid phase, and/or diffusion. A given chemical species is assumed to be in chemical equilibrium among the phases of a single compartment. However, there is no requirement for equilibrium between adjacent compartments. As an example of this process consider the upper soil layer. It is composed of three phases: soil water, soil matter, and soil gas. An organic chemical added to the soil distributes itself among these three phases in such a way that chemical and physical equilibria are achieved. Among the potential chemical pathways from the upper-soil compartment are liquid advection as a dissolved component of soil water run-off, solid advection in dust suspensions, and diffusion from soil gas to the atmosphere.

Decay and transformation processes in GEOTOX are modeled as first-order removal processes. Decay constants are used to account for radioactive decay, hydrolysis, photolysis, oxidation, biodegradation, sedimentation, and advection losses in the atmosphere. These constants treat each of these processes as first-order, irreversible transformations.

## Human-Exposure Model

The human-exposure and health-risk model links environmental concentrations to potential exposure pathways and lifetime health risk. Exposure is expressed as daily intake of a contaminant per unit body weight averaged over an individual's lifetime. Two age groups, adult and child, are assumed for the analysis.

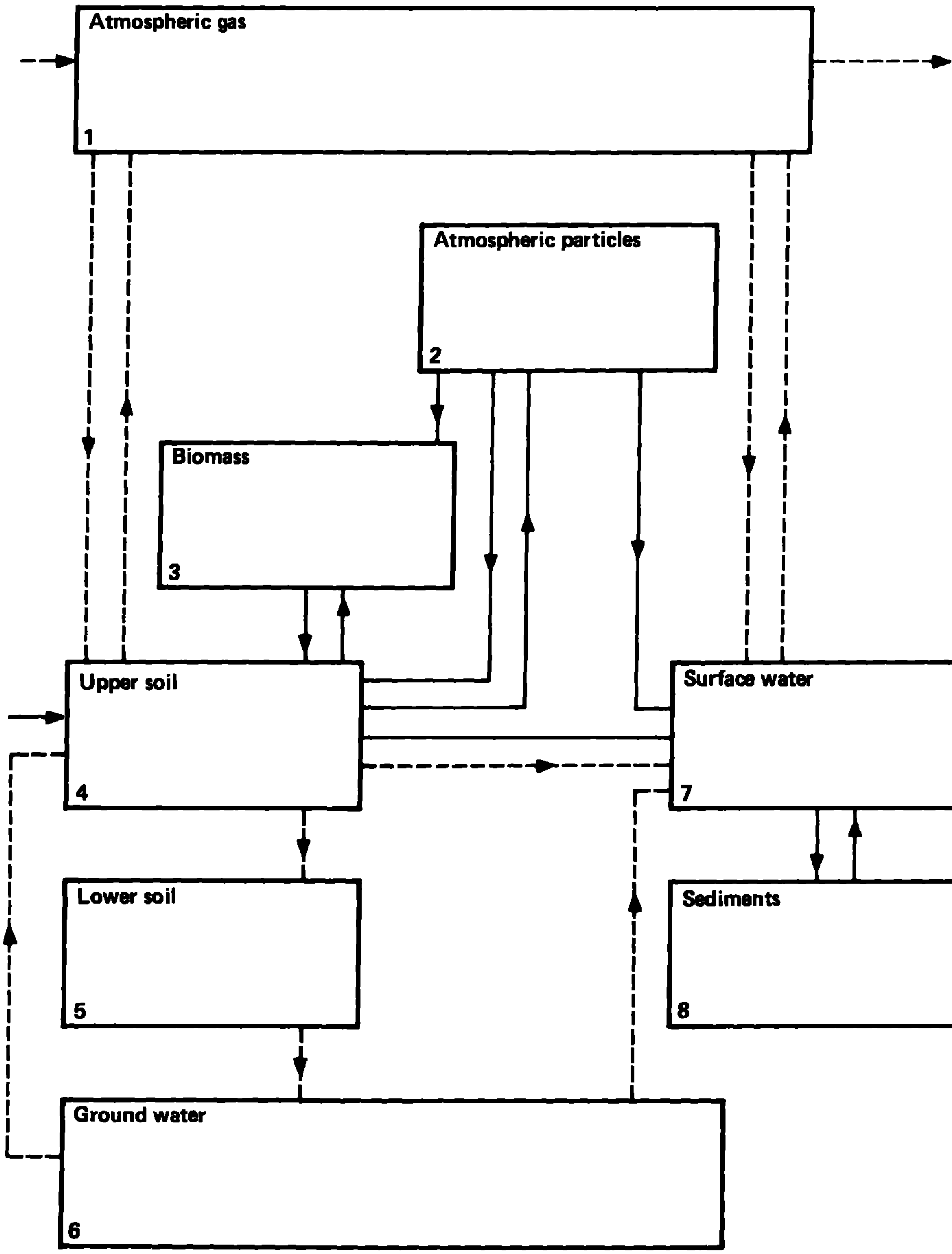


Figure 2. Interactions among the eight compartments in the GEOTOX model. Solid lines reflect the movements of dust and sediments; dotted lines reflect the movement of water.

Seven potential pathways are used in the analysis. These are (1) inhalation; (2) drinking water; (3) ingestion of fruits, vegetables, and grain; (4) ingestion of meat and dairy products; (5) ingestion of fish; (6) ingestion of soil; and (7) dermal absorption. Intake of a chemical by inhalation is the product of atmospheric concentration and breathing rate. Intake of a chemical through drinking water is the product of water concentration and daily water intake. Because roughly half of the water used in the U.S. comes from ground water, we assume the drinking-water supplies are split equally between surface and ground water. The intake of a chemical species through fruits, vegetables, and grains is the product of biota dry mass ingestion, the chemical concentration in soil, and a plant/soil partition coefficient. The remaining pathways involve more detailed assumptions that are dealt with in References 1 and 2.

Landscape and Chemical Data

In order to use the GEOTOX model to identify "high-priority" contaminants resulting from the open burning and open detonation of waste ordnance, we needed to prepare two sets of input data -- one for the properties of the landscapes or environments receiving the contaminants and the second for the properties of the contaminants. Because it was not feasible to develop parameter estimates for each of the landscapes associated with individual facilities processing waste ordnance, we group together those facilities that share basic environmental characteristics and use regional values for the input parameters. We used the national land-classification system developed for the Departments of Agriculture and Interior[13] as the basis for establishing groups. This system includes a number of ecosystem regions or ecoregions that are characterized by similar climate, soils, and natural biota. Thus, it is possible to determine representative regional values for the environmental parameters required to define the characteristics of the compartments that compose the model. Based on the geographic distribution of the various facilities processing waste ordnance, we defined three broad ecoregions. Figure 3 shows the location of the three major ecoregions along with the approximate location of the 15 major ordnance processing facilities.

The chemical properties that contribute to the intercompartment-transfer-rate constants are the chemical partition factors and diffusion coefficients. In order to run the GEOTOX model, we must know or estimate the solid/liquid partition coefficients between soil and soil water, ground water and aquifer material, and surface water and sediments; the air/liquid partition coefficient; the plant/soil partition coefficient; the fat/diet partition coefficient in cattle; and the bioconcentration factor in fish. We also need estimates of the diffusion coefficients of the substances in air and water.

The distribution of a chemical between solid and liquid is described with a sorption constant, $K_d$, that relates the amount of chemical sorbed to soil, rock, or sediment to the concentration in the water. The primary active surface that interacts with an organic chemical in the sorption process was shown to be the organic carbon fraction, $f_{oc}$, of the soil, rock, or sediment.[14] Therefore, the sorption characteristics of a chemical can be normalized to obtain a sorption constant based on organic carbon, $K_{oc}$, which is independent of the medium (i.e., soil, rock, or sediment).

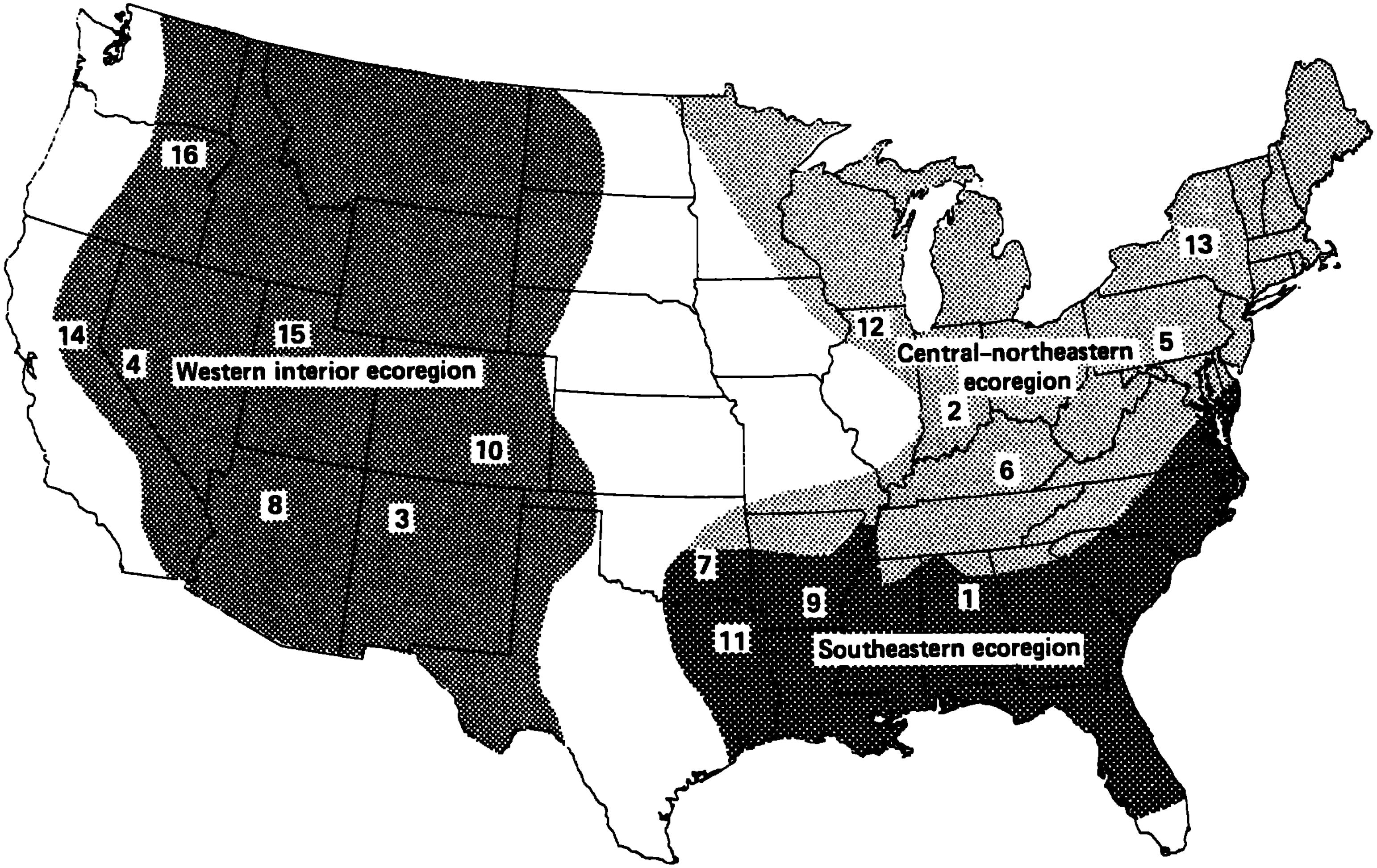


Figure 3. Geographical distribution of the three ecoregions with the approximate location of the 15 major ordnance-processing facilities.

$$K_d = K_{oc} \times f_{oc} , \tag{1}$$

$$K_{oc} = \frac{\text{mole/kg (carbon)}}{\text{mole/kg (water)}} . \tag{2}$$

The value of $K_{oc}$ can be derived from the several empirical relationships in which $K_{oc}$ is calculated as a function of properties such as water solubility.[14,15]

The plant/soil partition coefficient is obtained by assuming the water portion of the plant has the same concentration as soil water.[2]

The distribution of a chemical between water and air can be expressed using the Henry's law constant, H:

$$K_h = \frac{H}{RT} , \tag{3}$$

where

H = P/S, torr • kg/mole;
P = vapor pressure of the pure chemical, torr;
S = water solubility of the chemical, mole/kg (water);
R = gas constant, 62.4 torr • L/mole • K; and
T = temperature, kelvins (K).

## MULTIMEDIA TRANSPORT MODELS AND RISK ASSESSMENT/MANAGEMENT

The National Research Council divides the risk analysis process into two phases--risk assessment and risk management.[16] In addition to risk assessment and management, we should recognize that risk analysis usually begins with a hazard identification. Without the measurement or perception of a hazardous condition, there will be little or no effort to assess and manage risk. The object of risk assessment is to develop models and measures that can be used to determine the magnitude of the risk, parameters that contribute to this magnitude, and the likely uncertainty about the magnitude. Risk management is the process of weighing policy alternatives and selecting an appropriate institutional response. This process should integrate the results of risk assessment with engineering data and with social, economic, and political valuation to reach a decision. Linking these processes is the concurrent effort to evaluate risk. Risk evaluation directs the risk-assessment/management process in terms of individual and societal valuations of risk.

In this section we consider ways that multimedia models can be applied to risk assessment and management. In risk assessment, these models offer the analyst the potential to prepare a more comprehensive picture of the impact of toxic chemicals. In the risk-management area, these models provide a holistic framework, which, although incomplete, does offer decisionmakers an opportunity to compare a number of options for controlling risk.

## Multimedia Models and Risk Assessment

The comprehensive character of multimedia risk-assessment models makes them well-suited to sensitivity and uncertainty studies. These models can be used to compare the sensitivity of predicted human health risks to variabilities in chemical properties and environmental transport parameters. Using Monte-Carlo methods, the random variability of input parameters can be propagated through the models to determine the uncertainty in estimates of health risk. A stepwise regression analysis can be used to correlate the uncertainties in risk estimates to the uncertainty or random variability of specific input parameters.

There is no universally accepted method for the analysis of parameter uncertainty and sensitivity in multimedia-type systems models. However, there are a number of commonly used approaches. Uncertainty in model output results from the natural variability of real processes, measurement uncertainty associated with input parameters, and the exclusion and aggregation of processes in models. Sensitivity in models often refers to the rate of change of model output with respect to each input parameter.

Two general approaches are available for investigating the propagation of uncertainty in ecosystem-type models. For some (but very few) cases, the variability in model output can be estimated analytically. This is the case for models that can be either reduced to or approximated by a series of multiplicative parameters. For most cases, the output uncertainty must be estimated numerically using Monte Carlo techniques. Uncertainty studies using the GEOTOX code require this approach. The goal of the uncertainty analysis should be to identify the parameters that are influential in determining the variability in the output. In addition, we would like to determine the extent to which the overall variability is reducible.

The various approaches for sensitivity analysis are characterized by differences in the way they measure the influence of parameters on model output. A measure of sensitivity may be either local or global. A local measure is one that reflects the influence of small changes in the parameter values only in the region near the set of nominal or baseline values. A global measure reflects their influence over the entire range of values that the parameter may assume. A sensitivity analysis can incorporate the effects of interactions among parameters or it may require the assumption that no interactions exist. In determining the acceptability of contaminated food and water supplies, we use a global sensitivity analysis applied to the results of the uncertainty analysis. Mapping inputs to outputs using Monte Carlo techniques, followed by a simple stepwise regression, can be used to correlate the variability of individual input parameters with the variability in model predictions.

## Multimedia Models and Risk Management

In the paragraphs below we identify three ways that multimedia models contribute to the risk-management process. These are enhanced visualization, value of information, and flexible standards. In each case, the test of utility is to ask how the models can help the decisionmaker select among alternatives for managing risk. Often the decisionmakers must choose when to stop collecting more information. Because of this, the suitability of multimedia models for value-of-information studies may be their major contribution to the risk-management process.

Enhanced visualization is not just a qualitative feature but a quantitative feature of multimedia models. In assisting the regulation of toxic chemicals, these models provide a means for visualizing and quantifying the transfer of chemicals within the environment. For each chemical we can simulate how landscape and chemical properties affect the source/receptor/health-risk sequence. This type of information is quite useful to decisionmakers in both the public and the private sector.

Value-of-information refers to the value of increasing the precision of input parameters or the value of expanding models to include more state variables. In a risk assessment, the information provided by multimedia models provides the basis for exposure estimates. Exposure estimates using multimedia models are sequential. In the early phase of analysis an incomplete data base is used with simple models to estimate exposure and risk. As the analysis proceeds, more data may be collected and more complex models used. A critical issue in this process is how to determine when to stop refining the analysis, and recommend standards. Evans[17] suggests that a decisionmaker should collect additional information only when the value of the additional information exceeds the cost. We can estimate the cost of additional information. It is the cost of additional sampling, more chemical and physical analyses, and improved models. However, it is not as obvious how to determine the value of additional information. However, statistical decision analysis provides an analytical framework for estimating the value of information. Using this framework, one can determine when additional information would be beneficial. In general the test of information value is the extent to which new information will affect a decision. This "value-of-information" approach provides a guide to the development and improvement of multimedia models for use in risk assessment.

Flexible standards for exposure to toxic chemicals are risk-based standards that specify acceptable risk instead of specifying acceptable release rates. Such standards are flexible in the sense that the specified release rate varies with the assimilative capacity of the receiving compartment. Flexible standards allow variable treatment of releases based on the character of the ecoregion under consideration. However, standards of this sort could not be implemented without using multimedia models that handle chemical transport, exposure, and health risk in a precise and comprehensive manner.

## A SAMPLE APPLICATION

We have used GEOTOX to rank the potential health risks associated with ordnance residuals in the three ecoregions. These residuals result from open burning and open detonation of explosives. Six chemicals are included in the analysis. These are benzene; dibutyl phthalate; diethyl phthalate; hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX); 2,4-dinitrotoluene (DNT); and 2,4,6-trinitrotoluene (TNT). The screening is carried out in three steps.

First, we calculate the unit exposure that results from a continuous addition of 1 g-mole/km$^2$-yr of each chemical to each ecoregion. This exposure is compared to a virtually safe dose rate (VSDR). Next, we report the amount of each chemical that is produced annually as ordnance residuals in the U.S. and determine the fraction of this amount that is added to each ecoregion. Finally, we scale the unit exposure ranking by the relative fraction of each chemical added to each ecoregion in order to obtain a revised ranking based on the geographic fate of all domestic residuals.

Table 1 shows the results of the unit-exposure analysis, in which 1 g-mole/km$^2$-yr of each chemical is continuously added to the upper soil layer of each ecoregion. Exposures in mg/kg-d are summed over all seven pathways. The first column of Table 1 lists the six chemicals and the exposure pathways that account for the major fraction of the total exposure. Benzene exposure is dominated by inhalation. For DNT, inhalation and drinking-water ingestion account for most of the exposure. For the other four chemicals, drinking-water and food ingestion account for most of the exposure. Milk and meat ingestion, dermal absorption, and soil ingestion fail to appear as important pathways for this set of chemicals.

The next three columns in Table 1 give the average daily lifetime exposure that is estimated using GEOTOX. This reflects the exposure to individuals residing in and obtaining all of their air, food, and water from the contaminated landscape. The last column lists the VSDR for each chemical.

Table 2 lists quantities of each chemical that are projected to be produced annually in the U.S. as residues from ordnance destruction. Also listed is the relative fraction of these residues that is expected to end up in each ecoregion. We took the unit exposures in Table 1 and multiplied them by the corresponding quantities (mole/yr) and relative fractions to obtain the revised ranking in Figure 4. The resulting values are normalized so that the lowest value is near 1. Here, the ranking reflects not only the unit exposures but also the relative amount of each chemical discarded and the ecoregion receiving that chemical. Because of the amounts produced, DNT, RDX, and TNT become significantly more important than they were for the unit-exposure analysis.

## CONCLUSIONS

The process of identifying chemical residuals that should be the focus of data-base assessments includes three primary elements. These are the estimation of release rates into the environment, prediction of human doses based on the distribution of the by-products among environmental media, and finally, comparison of hypothetical doses against acceptable daily intakes. One goal of our ranking or screening procedure is to derive as much information as possible on each chemical in order to understand which compounds merit the greatest attention. One drawback to this scheme is that the lack of data on various contaminant parameters will affect the predicted risk of those contaminants. In addition, inadequacies in the modeling technique will also affect the risk ranking. We therefore consider these models as tools that assist our effort to identify and assess high-priority substances.

Table 1. Steady-state exposures that result from a continuous addition of one g-mole/km$^2$-yr to the upper soil of each ecoregion.

| Chemical (dominant pathways) in parentheses | Exposure (mg/kg-d) Southeast | Central-northeast | West | VSDR[a] (mg/kg-d) |
|---|---|---|---|---|
| Benzene (inhalation) | $3.4 \times 10^{-7}$ | $3.4 \times 10^{-7}$ | $3.4 \times 10^{-7}$ | $4.0 \times 10^{-5}$ [b] |
| Dibutyl phthalate (fish, drinking water, biota) | $3.5 \times 10^{-5}$ | $3.5 \times 10^{-5}$ | $7.9 \times 10^{-5}$ | $5.3 \times 10^{-2}$ [c] |
| Diethyl phthalate (drinking water, biota) | $1.7 \times 10^{-5}$ | $1.6 \times 10^{-5}$ | $2.5 \times 10^{-5}$ | $6.2 \times 10^{-2}$ [c] |
| RDX (biota, drinking water) | $4.5 \times 10^{-5}$ | $3.9 \times 10^{-5}$ | $1.6 \times 10^{-5}$ | $1.0 \times 10^{-2}$ [d] |
| TNT (drinking water, biota) | $2.0 \times 10^{-5}$ | $1.9 \times 10^{-5}$ | $5.8 \times 10^{-5}$ | $1.0 \times 10^{-3}$ [e] |
| DNT (inhalation, drinking water) | $1.1 \times 10^{-6}$ | $1.1 \times 10^{-6}$ | $1.1 \times 10^{-6}$ | $3.2 \times 10^{-5}$ [f] |

[a] Virtually safe dose rate.

[b] Dose rate for a lifetime leukemia risk of $10^{-6}$ (Ref. 18).

[c] Based on $LD_{50}$ in mouse[16] with a $10^{-5}$ safety factor.

[d] 90 d no effects level (NOEL) in monkey-feeding studies[19] with $10^{-2}$ safety factor.

[e] Derived from drinking-water standard.[20]

[f] Derived from water-quality criterion.[21]

We have illustrated the use of the GEOTOX model for ranking the potential exposures to a set of six chemicals. This ranking exercise indicates that DNT, TNT, and RDX require higher priority in future expansions of the data base for ordnance residues.

One of the larger data gaps we have identified involves the absence of a realistic approach to model or estimate the uptake by humans of organic chemicals through forage crops and edible plants. Because of this, we deal with plant uptake using a simple, and perhaps conservative, approach that

Table 2. The total annual release of six chemicals as ordnance residuals and their distribution by ecoregion.

| Chemical | Total release in residuals (mole/yr) | Fractional distribution by ecoregion | | |
|---|---|---|---|---|
| | | Southeast | Central-northeast | West |
| Benzene | 80 | 0.27 | 0.18 | 0.55 |
| Dibutyl phthalate | 160 | 0.32 | 0.21 | 0.47 |
| Diethyl phthalate | 26 | 0.20 | 0.46 | 0.34 |
| DNT | 590 | 0.32 | 0.22 | 0.46 |
| RDX | 2900 | 0.27 | 0.15 | 0.58 |
| TNT | 5700 | 0.28 | 0.18 | 0.54 |

assumes that the concentration in plant tissues is the same as that in soil-pore water. The utility of screening methods, such as the one in this paper, could be substantially enhanced by efforts to improve the modeling and understanding of soil-plant partitioning.

We have found that health risks from contaminants in a multimedia environment are sensitive to the magnitude of the source terms, acceptable daily doses, and environmental partitioning and residence time. Many compounds have a high potential risk because of uncertainties about one or more of these factors. In particular, the absence of information about environmental degradation could be responsible for overestimating potential health risks by orders of magnitude. The only way to reduce the uncertainty in these cases is to expand the data base on their environmental chemistry.

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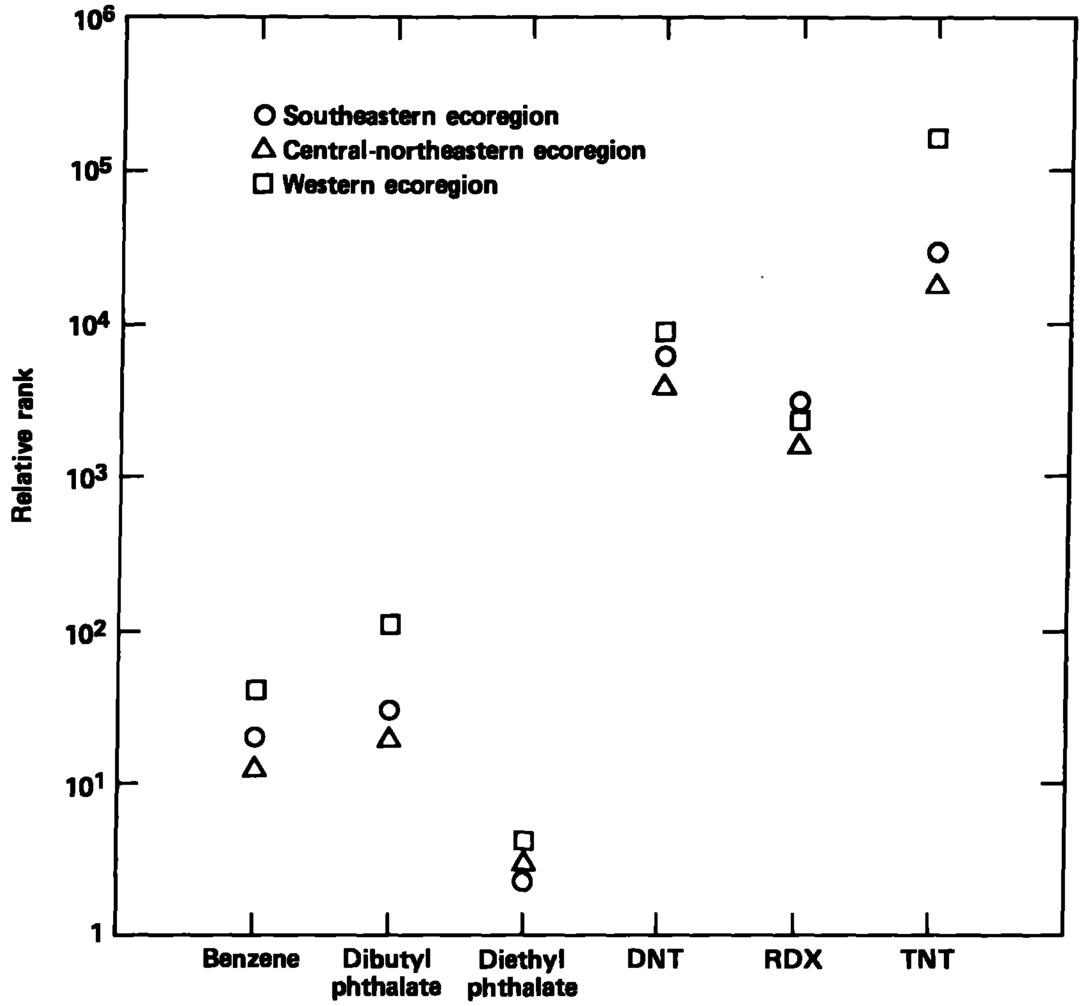


Figure 4. Relative rankings based on an adjustment of the unit-exposure analysis to account for the amount of each chemical generated and the ecoregion receiving it.

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